

Bohmian Mechanics with Complex Action: A New Trajectory-Based Formulation of Quantum Mechanics

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In recent years there has been a resurgence of interest in Bohmian mechanics as a numerical tool because of its local dynamics, which suggest the possibility of significant computational advantages for the simulation of large quantum systems. However, closer inspection of the Bohmian formulation reveals that the nonlocality of quantum mechanics has not disappeared — it has simply been swept under the rug into the quantum force. In this paper we present a new formulation of Bohmian mechanics in which the quantum action, S , is taken to be complex. This leads to a single equation for complex S , and ultimately complex x and p but there is a reward for this complexification — a significantly higher degree of localization. The quantum force in the new approach vanishes for Gaussian wavepacket dynamics, and its effect on barrier tunneling processes is orders of magnitude lower than that of the classical force. We demonstrate tunneling probabilities that are in virtually perfect agreement with the exact quantum mechanics down to 10^{-7} calculated from strictly localized quantum trajectories that do not communicate with their neighbors. The new formulation may have significant implications for fundamental quantum mechanics, ranging from the interpretation of non-locality to measures of quantum complexity.

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Ever since the advent of Quantum Mechanics, there has been a quest for a trajectory-based formulation of quantum theory that is exact. In the 1950's, David Bohm, building on earlier work by Madelung[1] and de Broglie[2], developed an exact formulation of quantum mechanics in which trajectories evolve in the presence of the usual Newtonian force plus an additional quantum force[3]. In recent years there has been a resurgence of interest in Bohmian mechanics (BM) as a numerical tool because of its local dynamics, which suggests the possibility of significant computational advantages for the simulation of large quantum systems[4, 5, 6, 7, 8, 9, 10, 11]. However, closer inspection of the Bohmian formulation reveals that the non-locality of quantum mechanics has not disappeared — it has simply been swept under the rug into the quantum force. Particularly disturbing is the fact that for simple cases such as Gaussian wave packet dynamics of the free particle or the harmonic oscillator, where classical-quantum correspondence should be perfect, the quantum force is not only non-vanishing but is the same magnitude as the classical force[12].

In this paper we present a new formulation of BM in which the quantum phase, S , is taken to be complex. This leads to a *single* equation for the complex phase, as opposed to coupled equations for real phase and real amplitude in the conventional BM. Complex phase leads to equations of motion for trajectories with complex x and p but there is a reward for this complexification — a significantly higher degree of localization than in conventional BM. We demonstrate tunneling probabilities that are in virtually perfect agreement with the exact quantum mechanics down to 10^{-7} calculated from strictly localized quantum trajectories that do not communicate with their neighbors. There is a superficial similarity

with some earlier work[13, 14] on a time-dependent extension of WKB, but the present approach, which we call Bohmian mechanics with complex action (BOMCA) is formally exact, and not semiclassical.

The starting point of conventional BM formulation (in 1-dimension) is the insertion of the ansatz

$$\psi(x, t) = A(x, t) \exp \left[\frac{i}{\hbar} S(x, t) \right], \quad (0.1)$$

in the time dependent Schrödinger equation (TDSE), where $A(x, t)$, $S(x, t)$ are *real* functions representing the amplitude and phase respectively. Separating the result into its real and imaginary parts, two PDE's are obtained

$$S_t + \frac{S_x^2}{2m} + V = \frac{\hbar^2}{2m} \frac{A_{xx}}{A}, \quad (0.2)$$

$$A_t + \frac{1}{m} A_x S_x + \frac{1}{2m} A S_{xx} = 0, \quad (0.3)$$

where $V(x)$ is the potential of the system. The first equation is referred to as the quantum Hamilton-Jacobi (HJ) equation; it differs from the classical HJ equation (the LHS) by the addition of a "quantum potential" $Q \equiv -\frac{\hbar^2}{2m} \frac{A_{xx}}{A}$. Defining a velocity field $v(x, t) = S_x(x, t)/m$ the classical HJ equation yields Newton's equation of motion; the same process for the quantum HJ equation yields equations of motion for "quantum trajectories". Eq.(0.3) can be reformulated as a hydrodynamic-like continuity equation for probability flow, hence eqs.(0.2) and (0.3) are referred to as the hydrodynamic formulation of quantum mechanics. The solution of the quantum hydrodynamic equations along the quantum trajectories constitutes the conventional BM formulation.

The starting point of the BOMCA formulation is the

insertion of the ansatz[12]

$$\psi(x, t) = \exp \left[\frac{i}{\hbar} S(x, t) \right], \quad (0.4)$$

in the TDSE, where we allow the phase to be *complex*. This yields a *single* newly defined quantum HJ equation

$$S_t + \frac{1}{2m} S_x^2 + V = \frac{i\hbar}{2m} S_{xx}, \quad (0.5)$$

where $Q \equiv -\frac{i\hbar}{2m} S_{xx}$ is the new quantum potential. Note that there is no expansion in powers of \hbar in the derivation, hence eq.(0.5) is an *exact* formulation of the TDSE which to the best of our knowledge has not been explored in the literature.

In the spirit of conventional BM our aim is to solve eq.(0.5) in the Lagrangian approach, that is, along quantum trajectories. A quantum trajectory is defined by

$$\frac{dx}{dt} = v(x, t); \quad v(x, t) \equiv \frac{1}{m} S_x(x, t). \quad (0.6)$$

Due to the definition of x as time dependent in eq.(0.6) we write the solutions of this equation as $x(t; x_0)$ where x_0 is the starting point of the trajectory. Unlike conventional BM, the complex value of S yields quantum trajectories $x(t; x_0)$ that evolve in the complex plane. As a consequence, the new formulation requires analytic continuation of the wavefunction and the phase to the complex plane. We consider only analytic potentials $V(x)$ therefor $v(x, t)$ is analytic in regions which do not contain nodes of $\psi(x, t)$. To obtain an equation of motion for $v(x, t)$ we take the spatial derivative of eq.(0.5) and apply eq.(0.6) to obtain

$$m(v_t + vv_x) - \frac{i\hbar}{2} v_{xx} = -V_x(x). \quad (0.7)$$

Identifying the expression in the round brackets as a Lagrangian time derivative ($\frac{d}{dt} = \frac{\partial}{\partial t} + v \frac{\partial}{\partial x}$) of v , transforms eq.(0.7) to a Newtonian-like equation of motion for the velocity

$$\frac{dv[x(t; x_0), t]}{dt} = \underbrace{-\frac{V_x}{m}}_{F_c/m} + \underbrace{\frac{i\hbar}{2m} v_{xx}}_{F_q/m}, \quad (0.8)$$

where we identify F_c , F_q as the classical and the quantum force respectively. The non-locality of quantum mechanics is manifested in the appearance of v_{xx} in the quantum force. This term prevents the first equation in (0.6) and eq.(0.8) from being a closed set.

As in conventional BM, the main difficulty lies in estimating the quantum force. We tackle this problem by taking iterated spatial partial derivatives of eq.(0.8). The result can be written after a short manipulation as

$$\frac{dv^{(n)}}{dt} = -\frac{V^{(n+1)}}{m} + \frac{i\hbar}{2m} v^{(n+2)} - \tilde{g}_n; \quad n = 0, \dots, \infty, \quad (0.9)$$

where $\tilde{g}_0 = 0$ and $\tilde{g}_n = \sum_{j=1}^n \binom{n}{j} v^{(j)} v^{(n-j+1)}$ for $n \geq 1$. The superscripts denote the order of a partial spatial derivative. The set of eqs.(0.9) and the first equation in (0.6) are now an infinite but closed set that describes a *fully local* complex quantum trajectory. If these equations tend to 0 as $n \rightarrow \infty$, we may obtain a numerical approximation by truncating the infinite set at some $n = N$, thus replacing eq.(0.8) with a system of $N + 1$ coupled ODEs. Since each individual equation in (0.9) depends on the consecutive $v^{(n+2)}$, the truncation is done by setting $v^{(N+1)} = v^{(N+2)} = 0$. The initial conditions for the $v^{(n)}$'s are given by

$$v^{(n)}(0; x_0) = \frac{1}{m} \frac{\partial^n S_x}{\partial x^n} \Big|_{x=x_0, t=0} = \frac{\partial^n}{\partial x^n} \left(-i\hbar \frac{\psi_x}{\psi} \right) \Big|_{x=x_0, t=0}, \quad (0.10)$$

where we applied the definition from (0.6) together with $S = -i\hbar \ln \psi$ that follows from eq.(0.4). $x_0 \in \mathbf{C}$ is an initial position of an arbitrary single trajectory. A similar iterative differentiation process was applied in conventional BM[5, 6, 7] yielding a more complicated set of coupled equations of amplitude and phase derivatives.

The relation $v = S_x/m$ identifies the *phase field* with an *action field* of the quantum trajectories. The equation of motion for the action along a trajectory is similar to its classical counterpart with the addition of the quantum potential

$$\frac{dS[x(t; x_0), t]}{dt} = S_t + vS_x = \frac{1}{2}mv^2 - V + \frac{i\hbar}{2}v_x. \quad (0.11)$$

Having x, v and v_x , the action along a trajectory is obtained simply by adding the integral of eq.(0.11) to the initial value $S(x_0, 0) = -i\hbar \ln[\psi(x_0, 0)]$. Inserting the action in eq.(0.4) yields the value of the wavefunction $\psi[x(t; x_0), t] = \exp \{ \frac{i}{\hbar} S[x(t; x_0), t] \}$ at position $x(t; x_0)$ in the complex plane.

To obtain the wavefunction on the real axis at time t_f , in principle we need to propagate a set of initial positions $\{x_{0j}\}$ such that $\{x_j(t_f; x_{0j})\} \in \mathbf{R}$ at a specified time t_f . Tracing back the initial positions from final positions resembles the computationally expensive "root search" problem familiar from the semiclassical literature. However, here a set of initial positions can be readily obtained. Suppose the initial positions are restricted to a region where $\frac{\partial}{\partial x_0} x(t_f; x_0) \neq 0$ and that the mapping of initial positions x_0 to final positions $x(t_f; x_0)$ is an analytic function. Then the inverse mapping $x \mapsto x_0(t_f; x)$ is also analytic. Consequently we can write

$$x_0(t_f, x_b) = x_0(t_f; x_a) + \int_{x_a}^{x_b} \frac{\partial x_0(t_f; x')}{\partial x'} dx', \quad (0.12)$$

where we are free to choose the final positions x_a, x_b and the integration contour. For simplicity, suppose we have found an initial condition x_0 such that $x_a = x(t_f; x_0) \in \mathbf{R}$. Varying $x_b \in \mathbf{R}$ and choosing the integration contour

to be the real interval between x_a and x_b , we obtain from eq.(0.12) a curve $x_0(t_f; x_b)$ of initial conditions that reach the real axis at t_f . This can be translated to a numerical scheme for generating initial positions that map to the vicinity of the real axis, by writing an iterative discrete equation based on eq.(0.12)

$$x_{0_{j+1}} = x_{0_j} + \frac{\delta x_{0_j}}{\delta x_j} \Delta x'; \quad j \geq 1 \quad (0.13)$$

where we define $\delta x_{0_j} \equiv x_{0_j} - x_{0_{j-1}}$ and $\delta x_j \equiv x_j(t_f; x_{0_j}) - x_{j-1}(t_f; x_{0_{j-1}})$. $\Delta x'$ is a small step along the real axis. Since the final positions are not exactly on the real axis an *interpolation* process is used to extract the complex phase along the real axis from the action values at the set of final positions $\{x_j(t_f; x_{0_j})\}$.

As a numerical example we consider the one-dimensional scattering of an initial Gaussian wavepacket $\psi(x, 0) = (2\alpha/\pi)^{1/4} e^{[-\alpha(x-x_c)^2 + \frac{i}{\hbar} p_c(x-x_c)]}$ from an Eckart potential $V(x) = D/\cosh^2(\beta x)$. We take $x_c = -0.7$, $\alpha = 30\pi$, $D = 40$, $\beta = 4.32$ and $m = 30$ (all units are atomic units). In Fig.1 we depict several complex quantum trajectories for the case of translational energy $E = p_c^2/2m = 0$, for $N = 1$. Note that the complex values of x and p allow the trajectories to "tunnel" through the barrier centered at $x = 0$. In Fig.2 (a) we compare the exact wavefunction at $t = .85$, $E = 50$ with the BOMCA results for truncation at $N = 1, \dots, 4$. Note that the transmitted part of the wavefunction is nearly converged for $N = 1$, suggesting that BOMCA will be very efficient for calculating tunneling probabilities. In Fig.2 (b) we consider the case of extremely deep tunneling — $E = 0$ — and focus on the transmitted part of the wavefunction. The method converges uniformly, and even for truncation at $N = 1$ the agreement with the exact results is excellent. It is interesting to contrast the equations for $N = 1$ with classical mechanics. For $N = 1$ there is no quantum force: the equations of motion are precisely the *classical* equations of motion

$$\frac{dx}{dt} = v; \quad \frac{dv}{dt} = -\frac{V_x}{m}, \quad (0.14)$$

albeit for complex x and v . There is however a nonzero quantum potential that gives an additional term to the action integral (cf. eq.(0.11)), where the term v_x fulfils

$$\frac{dv_x}{dt} = -\frac{V_{xx}}{m} - v_x^2 \quad (0.15)$$

(eq.(0.9) with $n = N = 1$). It is interesting to note that the defining equations for $N = 1$ (eqs. 0.14-0.15 and eq.(0.11)) have appeared previously in the literature, in the context of semiclassical methods [14, 15]; we emphasize that here they emerge only as a convenient truncation to an otherwise exact quantum formulation.

The asymptotic tunneling probability $T(E)$ is calculated by integrating the absolute square of the wavefunction for $x > 0$ at a sufficiently long time. In Fig.3

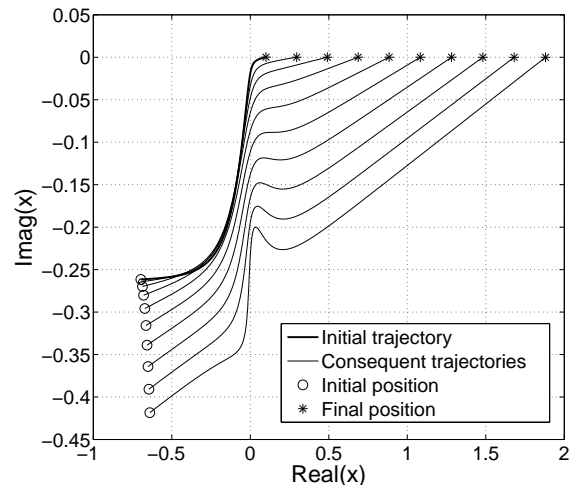


FIG. 1: Several complex quantum trajectories for the scattering of a Gaussian from an Eckart barrier centered around $x = 0$ where $E = p_c^2/m = 0$, $t = 1$ and $N = 1$. The trajectories were obtained through the numerical scheme described in the text (eq.(0.13)). Note that the trajectories initiate at $Re(x_0) \simeq -0.7 = x_c$ and reach $Re[x_f(x_0; t_f)] > 0$, $Im[x_f(x_0; t_f)] \simeq 0$. Hence, these trajectories "tunnel" through the barrier.

(a) and (b) we compare the exact tunneling probabilities as a function of E with the results obtained from BOMCA and conventional BM. The exact results were computed by a split operator wavepacket propagation. The BOMCA results were calculated by propagating 50 complex quantum trajectories. The conventional BM results were calculated using the numerical formulation developed by Lopreore and Wyatt[4]. The BOMCA formulation allowed the exploration of tunneling over the whole energy range, while the conventional BM formulation proved unstable at low energies ($E \lesssim 4$). Moreover, the BOMCA results are significantly more accurate than the BM results for all energies below the barrier height ($E < D$), even using just the classical equations of motion ($N = 1$). Note the improvement in the accuracy of the BOMCA results as N increases, suggesting convergence to the exact quantum result. The issue of convergence will be studied more fully in future work.

In summary we presented BOMCA, a novel formulation of Bohmian mechanics. This formulation yields simpler equations than conventional Bohmian mechanics (at the expense of complex trajectories). Moreover, BOMCA allows a direct and simple derivation of local uncoupled trajectories that may be used to reconstruct the wavefunction. The tunneling probabilities obtained by BOMCA for the scattering process were in excellent agreement with the exact results even in the extremely deep tunneling regime. We showed that even classical equations of motion with a small number of (complex)

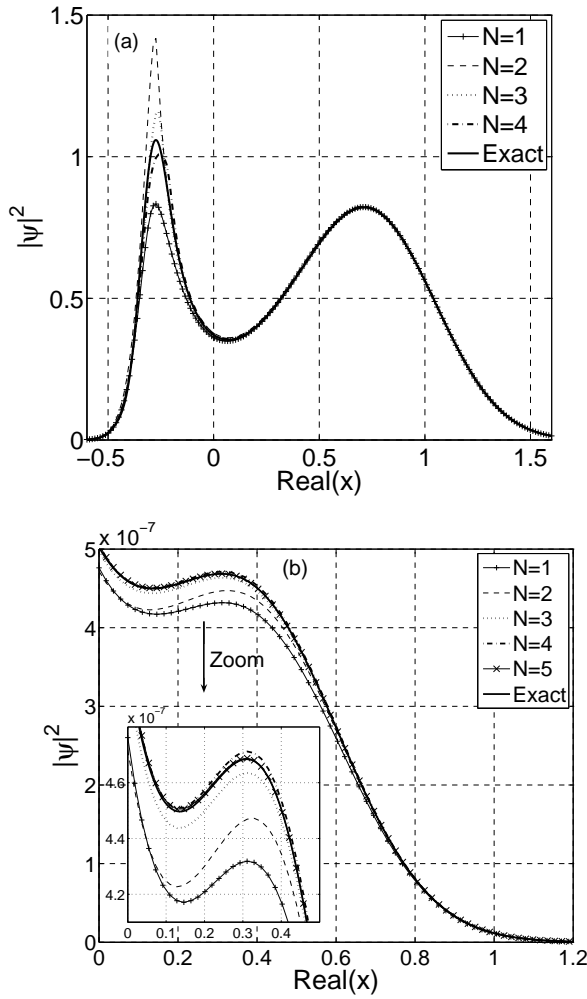


FIG. 2: Exact wavefunction vs. BOMCA reconstructed wavefunction for the scattering of a Gaussian from an Eckart barrier. Plot (a) corresponds to $t = 0.85$ and $E = 50$. Plot (b) focuses on the transmitted part of the wavefunction for the case of extremely deep tunneling — $t = 1$ and $E = 0$. Note the convergence to the exact wavefunction as N increases.

trajectories are sufficient to obtain very accurate results provided that an extra, nonclassical term is added to the action integral. We wish to acknowledge Prof. Edriss S. Titi for several useful discussions.

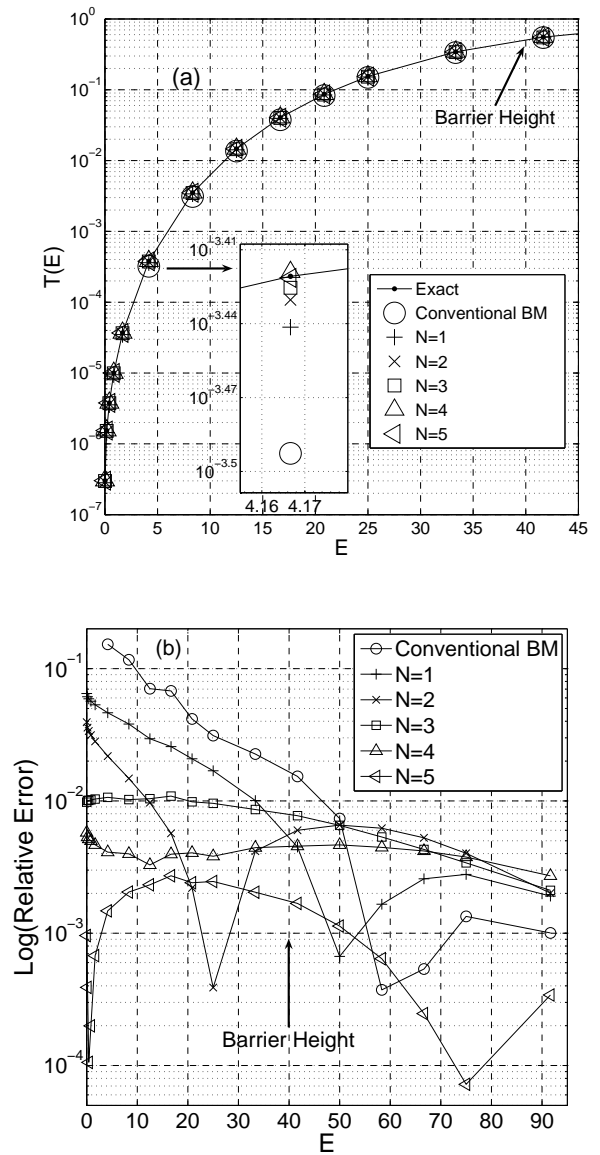


FIG. 3: (a) Comparison between the tunneling probabilities obtained by BOMCA, conventional BM and the exact results. The inset shows an enlargement of the results for $E \approx 4.17$, the last point for which the BM formulation was stable; for $E \lesssim 4$ we could not obtain stable results from the conventional BM formulation. (b) Log of the relative divergence from the exact results.

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